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THE MECHANISM OF PAIRING IN HUBBARD MOLECULES

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13. ABSTRACT *(Maximum 200 words)*

There exist many calculations for finite Hubbard clusters that do find pairing of electrons. At the same time, pairing is found to be absent in many other molecules. We have tried to find the mechanism of pairing by doing systematic calculations for a large number of Hubbard molecules. It is found that there exist two different mechanisms of pairing, corresponding to pairing occurring at small U (and vanishing at large U), and to pairing occurring only at large U. We find that the small-U pairing cannot be discussed without simultaneously discussing the Jahn-Teller distortions of the Hubbard molecules. Calculations that find pairing do so because they neglect the Jahn-Teller distortions of the molecules, and the pairing vanishes when the distortion is included in the model. The large-U pairing, surprisingly, is related neither to Jahn-Teller distortion nor to antiferromagnetism. Implications for high T_c oxides and doped C_{60} will be discussed.

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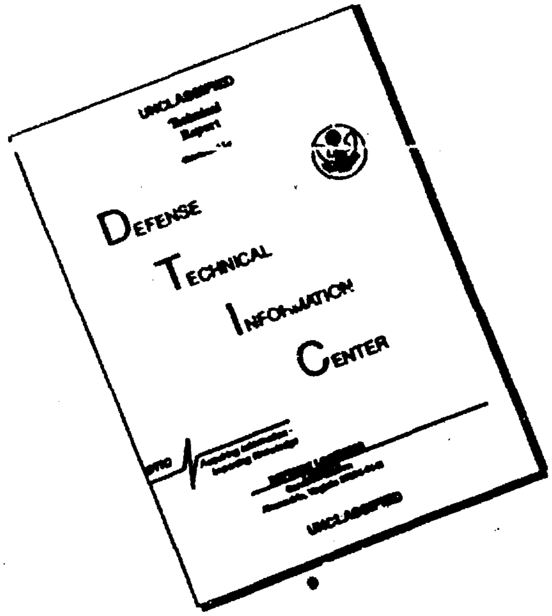

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9:36

M23 9 Doping dependence of the chemical potential in strongly correlated systems. M.B.J. MEINDERS, H. ESKES, G.A. SAWATZKY, University of Groningen (NL). — We calculated the one particle Green's function obtained by exact diagonalisations of one and two dimensional finite clusters for the Mott-Hubbard (MH) and charge-transfer (CT) models. We find that upon doping the insulator, the chemical potential shifts directly into the correlated band. There is no evidence for states moving into the gap. However, from k dependent calculations we find that for small electron (hole) doping concentrations and for bandwidths of the order of the Coulomb repulsion, some spectral weight appears in the gap which is due to the incoherent part of the one electron Green's function. At high doping concentration the gap between the lower and upper Hubbard band increases and the upper (lower) band loses most of its weight. It seems that the strongest changes occur in the spectral density upon doping due to a readjustment of spectral weights rather than a shifting around of states. This weight is transfered to states near the Fermi level.

9:48

M23 10 The mechanism of pairing in Hubbard molecules. S. MAZUMDAR and KIM-CHAU UNG, *U. Arizona*, and J.T. GAMMEL, *NCCOSC RDT&E Division (NRaD)* — There exist many calculations for finite Hubbard clusters that do find pairing of electrons. At the same time, pairing is found to be absent in many other molecules. We have tried to find the mechanism of pairing by doing systematic calculations for a large number of Hubbard molecules. It is found that there exist two different mechanisms of pairing, corresponding to pairing occurring at small U (and vanishing at large U), and to pairing occurring only at large U. We find that the small-U pairing cannot be discussed without simultaneously discussing the Jahn-Teller distortions of the Hubbard molecules. Calculations that find pairing do so because they neglect the Jahn-Teller distortions of the molecules, and the pairing vanishes when the distortion is included in the model. The large-U pairing, surprisingly, is related neither to Jahn-Teller distortion nor to antiferromagnetism. Implications for high T_c oxides and doped C_{60} will be discussed.

10:00

M23 11 DENSITY FUNCTIONALS FOR HUBBARD MODELS FROM THE FLUCTUATION-EXCHANGE APPROXIMATION. J.W. SERENE, *Complex Systems Theory Branch, Naval Research Laboratory, Washington, D.C. 20375-5345* - The fluctuation-exchange approximation was used to obtain a local approximation to the exchange-correlation free energy of the lattice version of Mermin's nonzero-temperature density functional theory.[1] for Hubbard hamiltonians with several choices of single-electron band structure. Results from these local density approximation were compared to results from the full fluctuation-exchange approximation for inhomogeneous two-band models.

[1] N.D. Mermin. Phys. Rev. 137, 1441 (1965).

Supplementary Papers

M23 12

Spin and Charge Dynamics in a 1D Two-Band Hubbard Model H.-Q. Ding and W.A. Goddard, CALTECH — A CuO_2 chain with one or two holes doped is studied via the 2-band Hubbard model in the large-U limit on a finite cluster. The quasiparticle band is $E_k = 0.87J\cos(2ka)$ with the bottom at $ka = \pi/2$. The quasiparticle are kinks which has the character of 3-spin polarons. The copper spin excitations are incommensurate spinwaves. The two doped holes repels each other very slightly, in contrast to the slight attraction in the t-J model. Spin-charge separation also occurs, as can be shown explicitly by using a Schwinger Boson representation.

[1] H.-Q. Ding and W.A. Goddard, Phys Rev.B January 1, 1992.

M23 13

Pseudogap Formation in the Half-filled Hubbard Model.* M. VEKIĆ, and S.R. WHITE, *UC Irvine* — Using quantum Monte Carlo, we study the evolution of pseudogaps in the spectral weight function for a half-filled two-dimensional Hubbard model as a function of temperature and coupling constant. The formation of pseudogaps at finite temperature can be used to distinguish between three regimes: 1) a strong coupling Mott-Hubbard regime, characterized by a pseudogap which persists even at high temperatures; 2) a weak-coupling spin-density-wave regime, characterized by the absence of a pseudogap at any finite temperature; and 3) an intermediate coupling regime with mixed behavior, characterized by a pseudogap that appears at a finite temperature.

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SESSION M24: DCMP: CALCULATIONS AND MODELING OF OPTICAL PROPERTIES

Thursday morning, 25 March 1993
Room 307 at 8:00
X. Zhu, presiding

8:00

M24 1 Explicit Determination of the Optical Matrix Elements from Empirical k-Space Hamiltonians. L. C. LEW YAN VOON, L. R. RAM-MOHAN[†], WPI, MA — We show that, contrary to popular belief, the optical matrix elements of a periodic solid can be explicitly calculated once the k-space Hamiltonian is known. *No additional parameters beyond those required to generate the band structure are needed.* Furthermore, the procedure does not involve numerical differentiation and integration. We illustrate the technique and present results for bulk semiconductors and superlattices described by a Slater-Koster Hamiltonian.

[†] Supported by the US Naval Research Laboratory (SDI-ISTO, Grant No. N00014-87-K-2031-LRR)

8:12

M24 2

Multipolar contributions to coherent optical second-harmonic generation at an interface between two isotropic media: A quantum-electrodynamical calculation. A. Wong and X.D. Zhu, University of California at Davis. Utilizing the Molecular Quantum Electrodynamics formalism, we revisited the bulk multipolar contribution to second-harmonic generation at the interface of two isotropic fluids.[1] The